Detonation Simulation Induced by Premixed H_2-Air Mixture Combustion

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1. Introduction

Hydrogen gas can be generated as a consequence of severe accident in a light water reactor. The hydrogen gas released from the reactor vessel is mixed with the air inside the containment building. The hydrogen-air mixture may lead to an explosion as the conditions are met. The explosion is called detonation and the effect of the impulsive mechanical load by the detonation might be serious to structural integrity of the containment building. The containment building plays a role of the last physical barrier to prevent the release of the radioactive materials to the environment. Therefore, the integrity of the containment building has to be kept intact even when the detonation wave blows it hard.

Shock waves generated by the detonation can be amplified or expanded when it propagates through internal structures inside the containment building. To protect the structures from the detonation, accurate numerical simulation models have to be developed. Numerical models to resolve the detonation induced by combustion of premixed hydrogen-air mixture should have capabilities of robust shock capturing as well as stable combustion modeling.

In this study, we utilized an OpenFOAM solver to simulate detonation phenomena. Numerical simulation model is validated through a shock tube test, detonation in a hemispherical balloon, and detonation in the RUT facility.

2. Methods and Results

2.1 Numerical Models

Numerical schemes for solving Riemann problems can be largely categorized into central schemes and upwind schemes. Roe's flux difference splitting family and van Leer's flux vector splitting family are famous upwind schemes. Upwind schemes are originated from the Godunov's scheme. On the other hand, Lax-Friedrichs scheme is a representative central scheme. Generally speaking, upwind schemes are more robust and accurate but complicated to implement because Riemann solver and characteristic decomposition are required. On the other hand, central schemes are simple but weak for strong shock and are known as more diffusive than upwind schemes especially in the discontinuity region.

Kurganov-Tadmor developed a second-order central-upwind semi-discrete KT scheme [1]. It can be considered as a descendant of the Lax-Friedrichs scheme. For general hyperbolic conservation laws which leads,

$$\frac{\partial w}{\partial t} + \frac{\partial F(w)}{\partial x} = 0, \tag{1}$$

with spatial variable x, conserved quantity w and flux F. Discretization of Eq. (1) by the semi-discrete KT scheme is expressed as,

$$\frac{d}{dt} w_j(t) = -\frac{H_{j+1/2}(t) - H_{j-1/2}(t)}{\Delta x}, \tag{2}$$

where, numerical flux H is written as

$$H_{i+1/2} = \frac{1}{2}\left[F\left(w^+_{i+1/2}\right) + F\left(w^-_{i+1/2}\right)\right] - \frac{1}{2} c_{i+1/2}\left[w^+_{i+1/2} - w^-_{i+1/2}\right]. \tag{3}$$

In Eq. (3), speed of propagation $c_{i+1/2}$ and reconstructed values $w^+_{i+1/2}, w^-_{i+1/2}$ of left and right faces at cell boundary $i + 1/2$ are defined as

$$c_{i+1/2} = \max\left(\left|\frac{\partial F}{\partial w}\left(w^-_{i+1/2}\right)\right|, \left|\frac{\partial F}{\partial w}\left(w^+_{i+1/2}\right)\right|\right) \tag{4}$$

$$w^+_{i+1/2} = \bar{w}^n_{i+1} - \frac{\Delta x}{2}(w_x)^n_{i+1} \tag{5}$$

$$w^-_{i+1/2} = \bar{w}^n_i + \frac{\Delta x}{2}(w_x)^n_i \tag{6}$$

where, $\bar{w}^n_i, (w_x)^n_i$ are cell averaged value and spatial derivative at time t^n and space x_i. Spatial derivatives are obtained by using slop limiters such as "minmod."

An OpenFOAM solver which implemented the KT scheme and is capable of solving chemical reaction was developed and named as "reactingPimpleCentralFoam." We applied a finite rate Arrhenius reaction model with a reduced hydrogen-air 7 step chemistry for combustion simulation [2]. Model constants are given in Table I [3] and were used for the simulations in Sec. 2.3 and 2.4.

Table I: Constants for H_2-Air 7-step reaction model [3].

n	reaction	A	β	$T_a = E_a/R_u$
1	$H_2 + O_2 = 2OH$	1.7×10^{10}	0	24233
2	$H + O_2 = OH + O$	1.42×10^{11}	0	8254
3	$H_2 + OH = H + H_2O$	3.16×10^{4}	1.8	1525
4	$O + H_2 = OH + H$	2.07×10^{11}	0	6920
5	$2OH = H_2O + O$	5.5×10^{10}	0	3523
6	$H + OH + M = H_2O + M$	2.21×10^{16}	-2	0
7	$2H + M = H_2 + M$	6.53×10^{11}	-1	0

2.2 1D Shock Tube Test

1D shock tube problem was selected to see that the OpenFOAM solver can resolve major characteristics of shock wave such as expansion fans, contact discontinuity, and shock. Initial conditions were set to the left side and the right side separated by a center position inside the shock tube. Pressure, density, velocity, and temperature conditions were given as follows

$$(P_L, \rho_L, U_L, T_L) = (100000, 1.0, 0, 298), \quad (7)$$
$$(P_R, \rho_R, U_R, T_R) = (10000, 0.1, 0, 298), \quad (8)$$

where the units of the properties are Pa, kg/m^3, m/s, K, respectively.

At the elapsed time of 7 ms, the density profiles are shown in Fig. 1 for which 100 grid points were used. For comparison, calculations utilizing 1st order accurate Roe scheme and 2nd order accurate upwind TVD scheme were also carried out. Three solvers can resolve well the propagation of shock, contact discontinuity, and expansion fan but it is figured out that Roe scheme's numerical dissipation smeared the shock more severely than the other two solvers. Grid refinement test with 400 grid points was performed and its result is shown in Fig. 2. The OpenFOAM solver gives comparable solution to the 2nd order upwind TVD scheme.

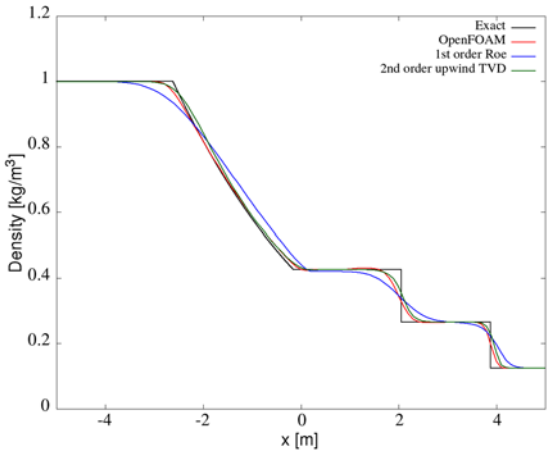

Fig. 1. Density profiles at 7 ms of shock tube problem with 100 grid points.

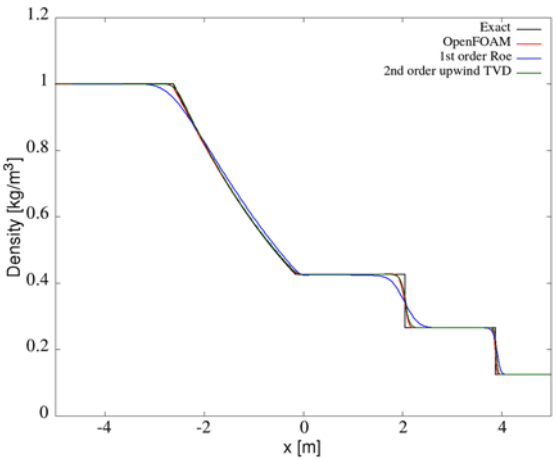

Fig. 2. Density profiles at 7 ms of shock tube problem with 400 grid points.

2.3 Detonation of Premixed H_2-Air Mixture in a Balloon

Experiments of detonation by premixed hydrogen-air mixture inside a hemispherical balloon was performed [4]. Initial condition of the mixture in the balloon are shown in Fig. 3. Along the path of moving shock, pressure sensors were mounted on the ground to measure the pressure peaks in the experiment [4]. Computational domain was discretized by 731,190 cells. Number of cells are composed of 9690 tetrahedral cells, 1500 polyhedral cells, and 720,000 hexahedral cells. Minimum and maximum face area are 1.87868e-5 m^2 and 2.62075e-2 m^2, respectively. Minimum and maximum cell volume are 1.24956e-7 m^3 and 4.07308e-3 m^3, respectively. Time step size was set to 1.e-8 s.

The mixture was ignited from the center of the balloon with 50 g of high explosive. Initial pressure field by hydrogen explosion was set by following equation,

$$\Delta p_m = \left[1.02 + \left(4.36 + 14\frac{m^{1/3}}{r}\right)\frac{m^{1/3}}{r}\right]\frac{m^{1/3}}{r} \text{ [bar]}, \quad (9)$$

where m, r are mass of explosive material and radius of the explosion, respectively [5].

Shock front passes through the balloon boundary between 10.8 ms and 11.2 ms. Fig. 4 shows pressure contours at 10.8 ms and 11.2 ms, respectively. We compared results using the OpenFOAM solver with data from the experiment which are shown in Fig. 5. Pressure profiles at the locations of 1.5 m and 2.75 m off the balloon center are obtained from the OpenFOAM solver with the Shang's reduced 7-step chemistry model. The OpenFOAM solver predicts detonation quite well.

A weak shock appears at 12.6 ms in the upper figure of Fig. 5. It was reported that a partial detonation shock was reflected from the hydrogen-air mixture/air interface at the balloon boundary [4]. The reflected shock moves inwardly and is superposed on the shock wave moving outwardly. It is why the pressure peak at 2.75 m simulated by the OpenFOAM becomes higher than that at 1.5 m by the OpenFOAM. This phenomenon is shown in Fig. 5.

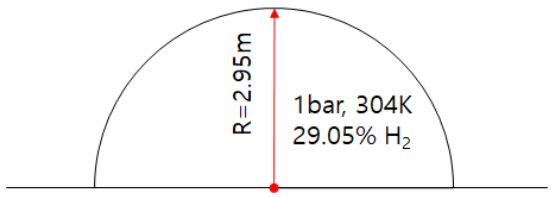

Fig. 3. Configuration of KIT hemispherical experiment.

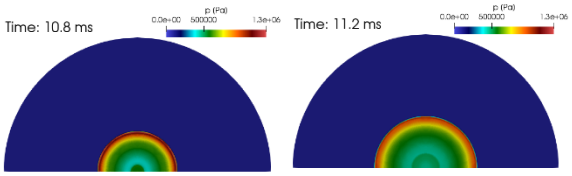

Fig. 4. Pressure contours at 10.8 ms (left) and 11.2 ms (right).

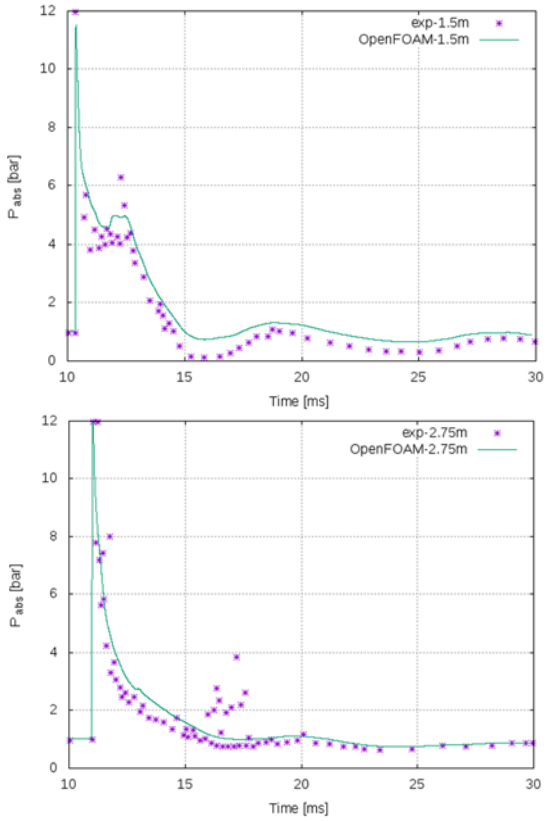

Fig. 5. Temporal history of simulated pressures at measuring locations of 1.5 m (top) and 2.75 m (bottom).

2.4 3D RUT Test

The OpenFOAM solver was also applied for 3D RUT benchmark problem to simulate complicated shock interactions induced by complex geometry of the RUT facility [6]. Among several experiments, KI-RUT-HYD09 was chosen for detonation simulation [6]. Mass fractions of hydrogen, oxygen, and nitrogen from 25.5% volume of hydrogen are 0.023, 0.225, 0.752, respectively. The ignition point is positioned at the end of the curved channel and is located 80 cm off from the floor and 50 cm off from the wall. Pressure was measured by pressure transducers located on the rear wall of the tunnel and the front wall of the canyon as shown in Fig. 6. In the experiment, 200 g high explosive charge was used for ignition.

For numerical simulation, computational domain was discretized with 2,211,900 hexahedral cells. Minimum and maximum face area are 1.38922e-3 m^2 and 3.98488e-3 m^2, respectively. Minimum and maximum cell volume are 5.90162e-5 m^3 and 1.97473e-4 m^3, respectively. Time step size was set to 1.e-8 s.

Detonation starts from the end of the curved channel as shown in Fig. 7. As time marches, complicated shock interactions appear as seen in Fig. 7. Shock waves reflect from side walls and form shock stems near the walls and expand when shock front enters into the canyon area. In Fig. 8, data from experiment and COM3D are compared with those obtained from the OpenFOAM solver at measuring points 11 and 8. Pressure peak is lower than the experiment but the OpenFOAM solver gives better results than COM3D [6].

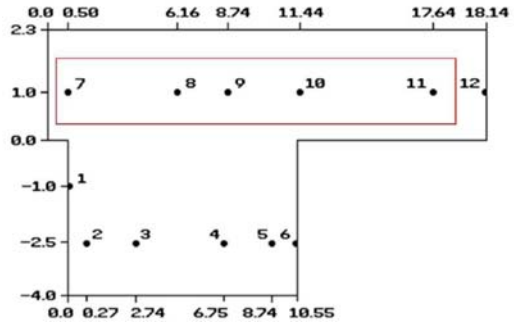

Fig. 6. Transducers to measure pressure.

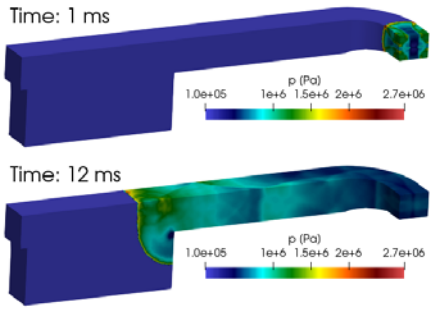

Fig. 7. Temporal histories of pressure at times of 1 ms (top) and 12 ms (bottom).

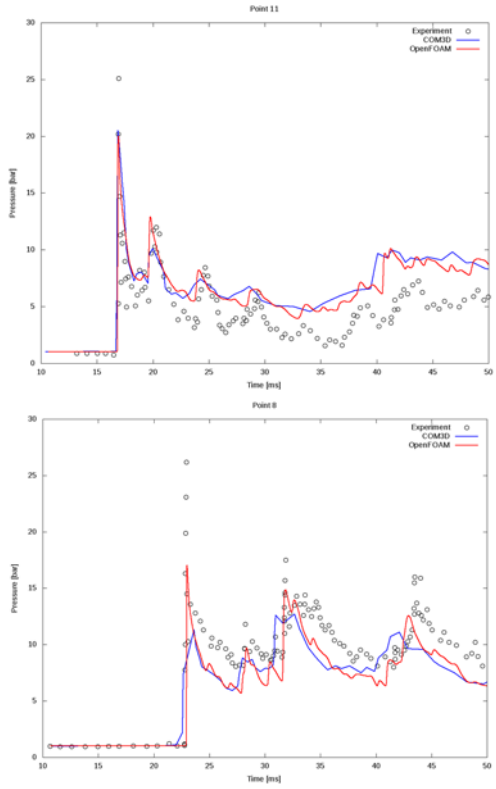

Fig 8. Temporal histories of pressures at measuring locations of 11 (top) and 8 (bottom).

Discrepancy between the experiment and the numerical simulations might be caused by ignoring of

support structures or by using coarse meshes near the rear wall. Through the channel and canyon areas, there were installed several support structures to protect the facility from the detonation, but for the simulations the detailed geometry couldn't be reflected due to absence of the geometrical data. When the shock wave passes through obstacles, the strength of the shock wave can be increased due to change of flow area but the OpenFOAM and COM3D simulations were carried out without reflecting such geometries. Another possibility is at using coarse meshes near the rear wall where the pressure sensors were mounted. Mach stems or reflected waves can be smeared with a coarse mesh near the wall.

3. Conclusion

Detonation phenomena accompanying chemical reactions have been simulated with an OpenFOAM solver with a reduced 7-step chemistry model and it was found out that the OpenFOAM solver can resolve complicated shock structures well. With respect to prediction errors of the OpenFOAM calculations, it can be concluded that the OpenFOAM predicted shock tube problem and detonation from a spherical balloon excellently but grid refinement tests with detailed geometrical modeling including support structures need to be supplemented for the RUT case.

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